Comparative exposure to DEHP from food contact materials: application of the product intake fraction

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Publication date:
2015

SETAC Europe 25th Annual Meeting
3-7 May 2015 | Barcelona, Spain

Environmental protection in a multi-stressed world: challenges for science, industry and regulators

BARCELONA 25
SETAC Europe 2015

ABSTRACT BOOK

ISSN 2309-8031

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SETAC Europe 25th Annual Meeting

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This book composes the abstracts of the presentations for the platform and poster sessions of the 25th Annual Meeting of the Society of Environmental Toxicology and Chemistry (SETAC), conducted at the International Congress Centre Barcelona (CCIB), in Barcelona, Spain from 3-7 May 2015. The abstracts are reproduced as accepted by the scientific committee of the meeting and appear in order of abstract code, in alphabetical order per presentation type. The poster spotlight abstracts are included in the list of poster abstracts. The presenting author of each abstract is underlined.

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the pre-action phase, body burdens showed no differences between younger and older adults. Therefore, cross-sectional sampling of a population is not required. In the post-action phase, simulations show different results depending on the intrinsic elimination half-life of a chemical. Rapidly eliminated chemicals showed the same pattern as in the pre-action phase, but clear age-concentration relationships could be observed for chemicals with slow elimination rates, where older adults have substantially higher body levels than young adults. Since intrinsic elimination is mostly unknown, it is recommended to sample cross-sectional during this phase in order not to potentially underestimate body levels for older adults. During this phase, it is also possible to evaluate the effectiveness of an action by estimating turn-off ages (the age where concentrations reach a plateau and cease to increase) in cross-sectional data. Modelling results revealed a key turn-off age of 25 + number of years after peak exposure, below which more aggressive actions to reduce exposure will likely result in lowering the overall body burden of the population further. At turn-off ages equal or higher than that value, further actions will have no significant effect on the population.

TH126

Comparative exposure to DEHP from food contact materials: application of the product intake fraction

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Food contact materials (FCM), e.g. bottles and food handling gloves, can contain potentially endocrine disrupting chemicals, such as di-2-ethylhexyl phthalate (DEHP, CAS: 117-81-7). To investigate the contribution of FCM to dietary DEHP exposure we apply the product intake fraction (PiF: g intake/g in product) – a metric accounting for human intake of chemical mass per unit of mass embodied within a product. PiF of ingestion of DEHP is estimated from empirical data for PET water bottles on the order of 1E-7 through 1E-5 and for food handling gloves from 1E-6 for rice and 1E-3 for radishes. The uncertainty is related to unknown information (chemical content in FCM), circumstances of use (e.g. food item), and any analytical uncertainty. Using PiF, maximum allowable concentrations of DEHP within water bottles and gloves were calculated with respect to regulatory thresholds. A hypothetical average PiF for the FCM sector was calculated via production volume and oral exposure doses estimated from NHANES data. In both cases the indication was gloves may contribute more to DEHP exposure when used with certain food items than bottled water. DEHP content in gloves greater than 5% would cause exceedance of US EPA threshold when used with certain food items, e.g. radishes based on PiF calculated here. The PiF used in thís context has applications for regulations related to FCM and exposure assessments on a per unit kilo basis.

TH127

Tissue dosimetry modeling of chemical mixtures containing Metals: a case study of Cd, Hg and Pb in humans

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Most of the current practices in the health risk assessments of exposures to chemicals and the subsequent regulatory measures are based upon data from studies on the individual chemical. However humans are simultaneously exposed to multiple xenobiotic chemicals (such as pharmaceuticals, metals, pesticides, volatile and semi-volatile organic compounds, etc.) that potentially possess a number of similar or different toxic effects. If more than one chemical enters the body, a potential arises for interactions among chemicals, their metabolites, and the biological molecules/systems. Consequently, the authorities are challenged to consider that this “chemical cocktail” or “total chemical load” does not produce unforeseen health effects. Combined action and interactions between chemicals, at high doses have been known for many years in the field of pharmacology. However, these in-situ experiences are not directly useful for predicting toxic effects of mixtures of environmental chemicals because the exposure levels of the general human population are relatively low and interactions occurring at high doses may not be representative for low-dose exposures. In case of toxic metals which are transported and eliminated through many common cellular mechanisms by "molecular mimicry" because of their similarities to essential metals, therefore, there exist toxicokinetic and toxicodynamic interactions among toxic and essential metals. Metal absorption, elimination, and toxicokinetics should therefore be considered highly correlated for exposed individuals, with susceptibilities resulting in differential effects of multiple metals. In this study, we analyse the toxicokinetic and toxicodynamic of Cd, Hg and Pb using generalized whole body physiologically-based pharmacokinetic (PBPK) models for a case study in Spain. Physiological variability in the population is considered across the model by linking with biological databases that provide physiological values for a majority of the tissues groups. Interaction effects between the study heavy metals mixtures are incorporated. Model has been validated with data from previous studies (1998-2007) of human exposure to metals in autopsy tissues of individuals living near a waste incinerator.

Effect Modelling of environmental systems - extrapolation and prediction of species response (P)

TH128

The use of dynamic population-level predictions in PERA: challenges and opportunities

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Population-level models are increasingly recognised as potentially powerful tools in environmental risk assessment. However, the practical application of dynamic population predictions for decision making is not straight forward in everyday risk assessment of down-the-drain chemicals. Probabilistic environmental risk assessment (PERA) has been suggested as a way to make uncertainty more explicit and to account for spatial and temporal variability. The outcome of a PERA is typically a measure of expected risk with an associated uncertainty interval. We present a conceptual framework that explores how probabilistic approaches can be applied in population models to incorporate more ecological relevance into risk assessments while keeping both uncertainty and variability explicit and transparent. One of the key challenges is understanding the protection goals for ecological scenarios exposed to anthropogenic stressors. For instance, systems that are already impaired by high volume emissions of untreated wastewater may require modified protection goals (e.g. protection of microbial purification processes and recovery of food web structure and diversity). For higher organisms, the protection goals must be reflected by a defined set of endpoint metrics that can quantify changes in population-level dynamics. These metrics must be carefully selected based on both the specific scenario and protection goal, as different options will lead to very different interpretations of effect. Finally we discuss the importance of making the relation between the willingness to accept risk and the severity of the effect explicit to facilitate decision-making. We consider these discussions a necessary first step in bringing the full potential of population-level models into risk assessment of down-the-drain chemicals.

TH129

Interspecies QAAR for pharmaceuticals

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Due to their extensive and progressive use in human and veterinary medicine, pharmaceuticals have been reported to be ubiquitously in surface and waste waters and are widely considered emerging environmental contaminants. Moreover, pharmaceuticals are specifically designed to be biologically active and their presence in the environment may be cause of serious concern for the wildlife. Even though a lot is known about pharmaceuticals’ human toxicity, there is a lack of knowledge about their potential environmental hazard and ecotoxicology. In-silico approaches, like those based on quantitative structure–activity relationships (QSARs), are valuable tools able to maximize the information contained in existing experimental data; in particular, quantitative activity-activity relationships (QAARs) allows to find out the interspecies correlations and to predict missing information extrapolating from one species to another. In this study we present different interspecies toxicity models between *Daphnia magna* and *Pimephales promelas*, between *Daphnia magna* and *Oncorhynchus mykiss* and between *the* two species of fish *Pimephales promelas* and *Oncorhynchus mykiss*,for the prediction of acute toxicity of many pharmaceuticals chemicals. In addition to the pure correlation QAARs, we also propose models based on species response and a selected molecular descriptor by the all-subset procedure included in QSARINS software, starting from a matrix of hundreds calculated 0D-2D descriptors by PaDEL-Descriptor software. All models presented are stable, robust and validated ($R2 > 0.75$ and $Q2loo > 0.70$) and can be used to extrapolate acute toxicity from and to different trophic levels. Particular attention was given to the structural applicability domain (AD) of the proposed models. We also analyzed the different correlations between the species, highlighting which ones were more correlated and which descriptors have more influence on them. Finally we applied the developed models to predict acute toxicity where data, for at least a species, were present and we compared the predictions derived from different models for the same chemical in order to propose consensus models to extrapolate information from crustacean to fish level.

TH130

Food web models as a tool for ecological scenario analysis

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One of the main challenges when evaluating the risk of a chemical for the environment is how to incorporate the large variation between and within ecological systems. A possible approach to deal with this diversity in biotic and abiotic conditions is to perform risk assessments for a selected set of possible scenarios. Standard scenarios cover a wide set of abiotic conditions e.g. spatial dimensions, hydrodynamics, physicochemical properties of chemicals and emission characteristics. Biological attributes also need to be accounted for e.g. the

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